

Autonomous ToF-SIMS Studies with AI-Agent Quality Control

Anton V. Ievlev, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory — Supplemental figures

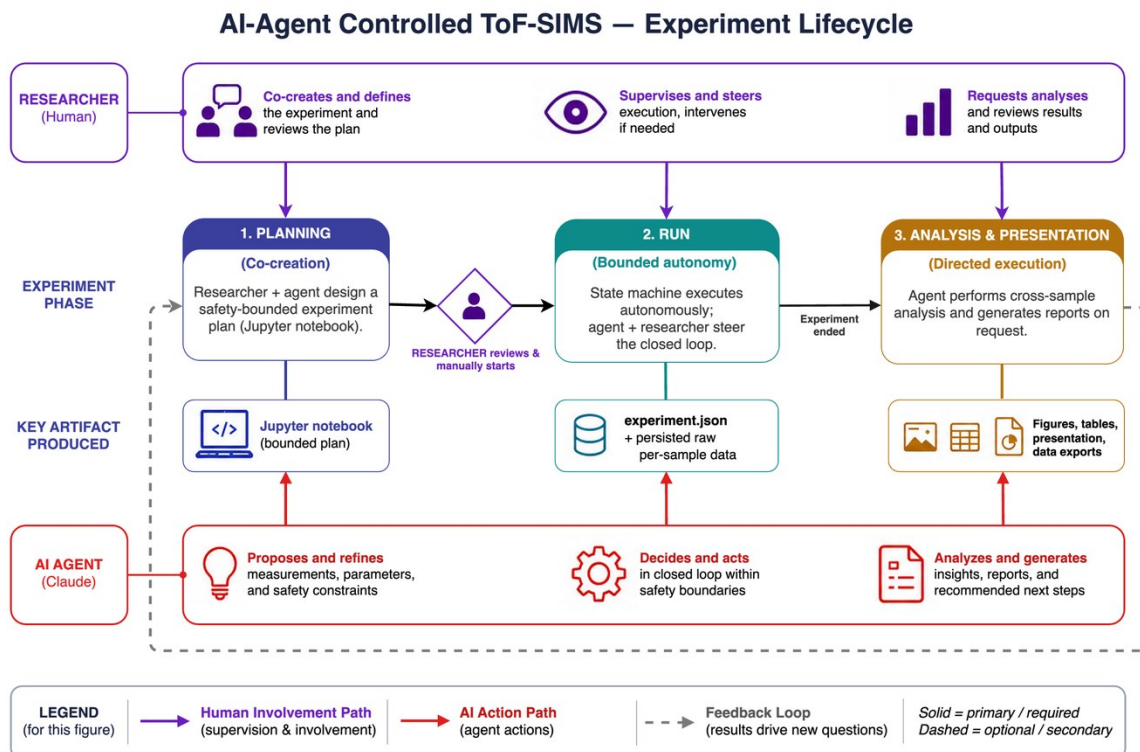


Fig. 1. The PACE-SIMS experiment lifecycle. In the planning phase, the researcher and the AI agent co-create a safety-bounded experiment plan captured as a Jupyter notebook; execution starts only after the researcher's manual go/no-go review. During the run, a state machine executes the plan autonomously while the agent decides and acts in a closed loop within human-approved safety boundaries, writing its decisions and the persisted raw per-sample data to a shared experiment state; the researcher supervises and can intervene. After the run, the agent performs cross-sample analysis and produces figures, tables, and reports on request. Purple arrows: human involvement; red: agent actions; dashed: feedback of results into new questions.

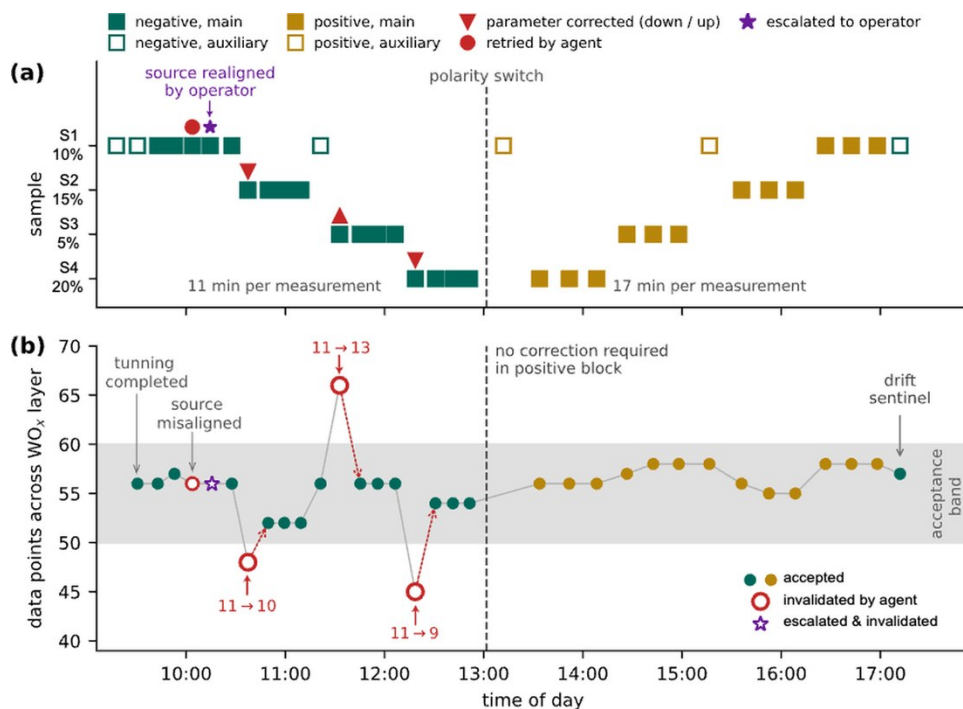


Fig. 2. Acquisition timeline of the blind two-polarity validation run (35 measurements, 8.1 h, ~40 min of total human attention). (a) Measurement sequence with agent decisions marked: parameter corrections, an agent-initiated retry, and one escalation to the operator for primary-beam source realignment. (b) Data points across the WO_x layer per measurement: the agent recalibrated per-sample sputter settings (11 → 10, 13, 9 frames) to hold sampling within the pre-agreed acceptance band; converged settings differed by 44% across the four films, and the drift sentinel closed the session.